Fate Report for Case # P-18-0219

Fate
Summary Statement

Fate Summary Statement: P-18-0219
FATE:
MW = [redacted] with [redacted] < 500 and [redacted] < 1000
[redacted] with MP < 25 °C
(E)
S = Reacts
Hydrolysis half-life = hr-da
VP < 1.0E-6 torr
at 25 °C (E)
BP > 400 °C (E)
H < 1.00E-8 (E)
POTW removal
(%) = PMN 90 via hydrolysis; then Hyd Pdt 90 via sorption
Time for
complete ultimate aerobic biodeg = Hyd Pdt > mo
Sorption to
soils/sediments = Hyd Pdt v.strong
PBT Potential: PMN P1B1; Hyd Pdt
P3B1
*CEB FATE: Migration to ground water = Hyd Pdt negl

PMN
Material:
Overall wastewater treatment removal is 90% via hydrolysis
(hydrolysis half-life: hours to days).
PMN Material:
Low
Persistence (P1) is based on hydrolysis of the parent compound (hydrolysis half-life: hours to days).
Low Bioaccumulation potential (B1) is
based on hydrolysis of the parent compound (hydrolysis half-life: hours to days).
Hydrolysis Product:
Overall wastewater treatment removal is
90% via sorption.
Sorption to sludge is strong based on data for [redacted]
[redacted] polymers.
Air Stripping (Volatilization to air) is
negligible based on data for [redacted] polymers.
Removal
by biodegradation in wastewater treatment is negligible based on data for

[redacted] polymers.
The aerobic aquatic biodegradation
half-life is greater than months based on data for [redacted]
polymers.
The anaerobic aquatic biodegradation half-life is greater
than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life.
Sorption to soil and
sediment is very strong based on data for [redacted] polymers.

Migration to groundwater is negligible based on data for [redacted]
[redacted] polymers.
Hydrolysis Product:
High Persistence
(P3) is based on the aerobic and anaerobic biodegradation half-lives.

Low Bioaccumulation potential (B1) is based on data for [redacted]
[redacted] polymers and low water solubility, which inhibits bioavailability and biodegradation.
Bioconcentration/Bioaccumulation factor to be
put into E-Fast: N/A.

[redacted]

Fate Assessor: Lee, Mari

SMILES: [redacted]

Physical Properties

Property	Measured/Calculated Value	EPI
Molecular Form:	[redacted]	
Molecular Wt.:	[redacted]	
% < 500:	[redacted]	
% < 1000:		

Property	Measured/Calculated Value	EPI

Property	Measured Value	Method	Estimated Value	Method	EPI
Melting Point:					
Boiling Point:			>400		
BP Pressure:					
Vapor Pressure:			<0.000001		
Water Solubility:			Reacts		
Log P:					
Log Kow:					
Log Koc:					
Log BCF:					
Henry's Law:					

pH:	
pH Comment:	

Fate Analysis

Hydrolysis (t1/2, da):	Volatilization (t1/2) - River (hr):	Volatilization (t1/2) - Lake (da):
Atm Ox Potential (t1/2)OH (hr):	Atm Ox Potential (t1/2)O3 (hr):	Atm Ox Potential (t1/2) Total (hr):
MITI Linear:	MITI NonLinear:	
Biodeg Linear:	Biodeg NonLinear:	
Biodeg Survey ult:	Biodeg Survey Prim:	
STP (% removal) Total:	STP (% removal) Biodeg:	

STP (% removal) Ads:	**STP (% removal) Air:**

Rationales

Removal in Wastewater Treatment:	
Atmospheric Oxidation:	
Hydrolysis:	
Photolysis:	
Aerobic Biodegradation:	
Anaerobic Biodegradation:	
Sorption to Soil and Sediment:	
Migration to Groundwater:	
Persistence - Air:	
Persistence - Water:	
Volatilization from Water:	
Soil:	
Sediment:	
Other:	
Standard:	
Bioaccumulation:	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	PBT Comments
1	1		PMN
3	1		Hyd Pdt

Exposure-Based Testing

Exposure-Based Testing:	

Fate Ratings
Removal in WWT/POTW (Overall):

Removal in WWT/POTW (Overall):	90;90 PMN;Hyd Pdt

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
WWT/POTW Sorption:	;3	Low	Moderate	Strong	V. Strong	PMN;Hyd Pdt
WWT/POTW Stripping:	;4	Extensive	Moderate	Low	Negligible	PMN;Hyd Pdt
Biodegradation Removal:	;4	Unknown	High	Moderate	Negligible	PMN;Hyd Pdt
Biodegradation Destruction:		Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	;4	<= Days	Weeks	Months	> Months	PMN;Hyd Pdt
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	;4	<= Days	Weeks	Months	> Months	PMN;Hyd Pdt
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Hydrolysis (t1/2 at pH 7,25C) A:	2-3	<= Minutes	Hours	Days	>= Months	-N=C=O
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	;1	V. Strong	Strong	Moderate	Low	PMN;Hyd Pdt
Migration to Ground Water:	;1	Negligible	Slow	Moderate	Rapid	PMN;Hyd Pdt
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
		Negligible	Slow	Moderate	Rapid	

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
Atmospheric Ox B, O3:						

Bio Comments:

Bio Comments:	The isocyanate groups are expected to hydrolyze with a half-life of hours to days, to give the amine-terminated polymer.

Fate Comments:

Fate Comments:	

Comments/Telephone Log

Artifact	Update/Upload Time